

Cellerator Arrow Quick Reference[†]

Cellerator Arrow	Name, <code>interpret[]</code> format, Differential Equations	Typical Biochemical Notation and other notes
$S \rightarrow P$	Conversion: <code>interpret[{{S → P}, k}, ...]</code> $\frac{dP}{dt} = kS, \frac{dS}{dt} = -kS$	$S \xrightarrow{k} P$
$A + B \rightarrow C$	Unidirectional: <code>interpret[{{A + B → C}, k}, ...]</code> $\frac{dA}{dt} = -kAB, \frac{dB}{dt} = -kAB, \frac{dC}{dt} = kAB$	$A + B \xrightarrow{k} C$
$A + B^n \rightarrow C$	Cooperative Unidirectional: (n must be an integer) <code>interpret[{{A + B^n → C}, k}, ...]</code> $\frac{dA}{dt} = \frac{dB}{dt} = -kAB^n = -k \frac{dC}{dt}$	$A + nB \xrightarrow{k} C$
$A_1 + A_2 + \dots \rightarrow B_1 + B_2 + \dots$	General Conversion: $\frac{dB_i}{dt} = -\frac{dA_i}{dt} = kA_1A_2A_3\dots A_n$	$A_1 + A_2 + \dots + A_n \xrightarrow{k} B_1 + B_2 + \dots + B_m$
$A \rightleftharpoons B$	Bidirectional Conversion: <code>interpret[{{A ⇌ B, kf, kr}, ...}]</code> $\frac{dA}{dt} = -\frac{dB}{dt} = -k_f A + k_r B,$	$A \xrightleftharpoons[k_r]{k_f} B$
$A + B \rightleftharpoons C$	Bidirectional: <code>interpret[{{A + B ⇌ C, kf, kr}, ...}]</code> $\frac{dA}{dt} = \frac{dB}{dt} = -\frac{dC}{dt} = -k_f AB + k_r C,$	$A + B \xrightleftharpoons[k_r]{k_f} C$
$\emptyset \rightarrow A$	Creation: <code>interpret[{{∅ → A, k}, ...}]</code> , $\frac{dA}{dt} = k$	$\emptyset^k \rightarrow A$
$A \rightarrow \emptyset$	Annihilation: <code>interpret[{{A → ∅, k}, ...}]</code> , $\frac{dA}{dt} = -kA$	$A \xrightarrow{k} \emptyset$
$\overset{E}{S \rightleftharpoons P}$	Catalytic*: <code>interpret[{{S ⇌ P, kfkr, k}, ...}]</code> $\frac{dS}{dt} = -k_f SE + k_r X, \frac{dP}{dt} = kX,$ $\frac{dX}{dt} = -\frac{dE}{dt} = k_f SE - (k + k_r)X$	$S + E \xrightleftharpoons[k_r]{k_f} X \xrightarrow{k} E + P$
$\overset{E}{S \rightleftharpoons P} \underset{F}{\rightleftharpoons}$	Bidirectional Catalytic*: <code>interpret[{{S ⇌ P, a1, d1, k1, a2, d2, k2}, ...}]</code> $\frac{dS}{dt} = a_1 SE + d_1 X + k_2 Y, \frac{dP}{dt} = k_1 X - a_2 PF + d_2 Y$ $\frac{dE}{dt} = -a_1 SE + (d_1 + k_1)X = -\frac{dX}{dt},$ $\frac{dF}{dt} = -a_2 PF + (d_2 + k_2)Y = -\frac{dY}{dt}$	$S + E \xrightleftharpoons[d_1]{a_1} X \xrightleftharpoons[k_2]{a_2} F + S$ $P + F \xrightleftharpoons[d_2]{k_1} Y \xrightleftharpoons[k_2]{a_2} E + P$ Equivalent to the set $\overset{E}{S \rightleftharpoons P}, \underset{F}{P \rightleftharpoons S}$
$\overset{E}{S \rightarrow P}$	Simplified non-saturating catalytic*: <code>interpret[{{S → P, k}, ...}, ...]</code> , $\frac{dP}{dt} = \frac{dS}{dt} = kES$	$S + E \xrightarrow{k} P + E$

* The variable "E" is used for illustrative purposes only, and should be avoided. Mathematica assigns a value of 2.718... to the symbol E.

$E \xrightarrow{A} B$	<p>Simplified Saturating Catalytic*:</p> $\text{interpret}\left[\{\{A \mapsto B, \text{type} \square \text{ hill}, \text{options}\}, \dots\}\right]$ $\frac{dB}{dt} = \frac{(k_0 + kE)A^n}{K_M^n + A^n} = \square \frac{dA}{dt}$ <p>Options[hill]= {vmax\square 1,nhill\square 1,khalf\square 1,basalRate\square 0} In this example: vmax\square k, basalRate\square k₀, khalf\square K_M, nhill\square n * The variable "E" is used for illustrative purposes only, and should be avoided. Mathematica assigns a value of 2.718... to the symbol E.</p>	<p>Gives Michaelis-Menten kinetics when $k_0 = 0$. Equivalent to $A \rightleftharpoons B$ under the assumptions that (1) the concentration of intermediate (X) is steady state; (2) that E represents total (free plus bound) enzyme, (3) that $K_M = (k + k_r) / k_f$, and (4) the basal rate $k_0 = 0$.</p>
$A \mapsto B$	<p>Hill-function regulation of B by A:</p> $\text{interpret}\left[\{\{A \mapsto B, \text{type} \square \text{ hill}, \text{options}\}, \dots\}\right] \text{ or } \text{interpret}\left[\{\{A \mapsto B, \text{hill}[\text{options}]\}, \dots\}\right]$ $\frac{dB}{dt} = r_0 + \frac{r_1 + vA^n}{k^n + A^n}, \quad \frac{dA}{dt} = 0$ <p>Options[hill]= {vmax\square 1,nhill\square 1,khalf\square 1,basalRate\square 0} In this example: vmax\square v, basalRate\square {r₀,r₁}, khalf\square K_M, nhill\square n If basalRate is an Atom it is used for r₀ and r₁</p>	<p>The set $\{A_i \mapsto B\}$, $i = 1, 2, \dots, p$, is interpreted as:</p> $\frac{dB}{dt} = r_0 + \frac{\left(r_1 + \prod_{i=1}^p v_i T_i A_i\right)^n}{k^n + \left(r_1 + \prod_{i=1}^p v_i T_i A_i\right)^n}$
$A \mapsto B$	<p>GRN-function Regulation of B by A:</p> $\text{interpret}\left[\{\{A \mapsto B, \text{GRN}[\text{options}]\}, \dots\}\right] \text{ or } \text{interpret}\left[\{\{A \mapsto B, \text{type} \square \text{ GRN}, \text{options}\}, \dots\}\right]$ $\frac{dB}{dt} = \frac{R}{1 + e^{\square T A^n + h}}$ <p>Options[GRN]= {RGRN\square 1,TGRN\square 1,nGRN\square 1,hGRN\square 0} In this example, RGRN\square R, TGRN\square T, nGRN\square n, hGRN\square h</p>	<p>The set $\{A_i \mapsto B\}$, $i = 1, 2, \dots, p$, is interpreted as:</p> $\frac{dB}{dt} = \frac{R}{1 + e^{\prod_i T_i A_i^{n_i} + h_i}}$
$(A_1, A_2, \dots) \mapsto C$	<p>Allosteric dynamics (NHCA)*, regulation of B by A: $\text{interpret}\left[\{\{A \mapsto B, \text{NHCA}[\text{options}]\}, \dots\}\right]$ or $\text{interpret}\left[\{\{A \mapsto B, \text{type} \square \text{ NHCA}, \text{options}\}, \dots\}\right]$</p> $\frac{dB}{dt} = \frac{(1 + T^\pm A^n)^m}{k(1 + T^\square A^n)^m + (1 + T^\pm A^n)^m}$ <p>If TNHCA is specified, use $T^\pm = \pm T \square (\pm T)$, otherwise T^\pm are given by TPLUS, TMINUS</p> <p>Options[NHCA]= {TPLUS\square 1,TMINUS\square 1,nNHCA\square 1,kNHCA\square 1,mNHCA\square 1,TNHCA\square {}} In the example, TPLUS\square T⁺, TMINUS\square T⁻, nNHCA\square n, mNHCA\square m, kNHCA\square k If NHCAmode\square 1 in options, $\frac{dB}{dt} = \frac{k T^\square A^n (1 + T^\square A^n)^{m\square 1} + T^\pm A^n (1 + T^\pm A^n)^{m\square 1}}{k(1 + T^\square A^n)^m + (1 + T^\pm A^n)^m}$</p> <p>* Non-Hierarchical Cooperative Activation. The (+) and (-) in the superscript are used for illustrative purposes only here; they will lead to confusion in Mathematica and should be avoided.</p>	<p>The set $\{A_i \mapsto B\}$, $i = 1, 2, \dots, p$, is interpreted as:</p> $\frac{dB}{dt} = \frac{\prod_i (1 + T_i^\pm A_i^{n_i})^m}{k \prod_i (1 + T_i^\square A_i^{n_i})^m + \prod_i (1 + T_i^\pm A_i^{n_i})^m}, \text{ or}$ $\frac{dB}{dt} = \frac{\prod_i (1 + T_i \square (T_i) A_i^{n_i})^m}{k \prod_i (1 \square T_i \square (T_i) A_i^{n_i})^m + \prod_i (1 + T_i \square (T_i) A_i^{n_i})^m}$